Synthesis, X-ray Structures and Hirshfeld Analysis of Two Novel Thiocyanate-Bridged Ag(I) Coordination Polymers

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Table. S1. Crystal data and structure refinement for complexes **1** and **2**.

	1	**2**
CCDC	2298037	2298038
Empirical formula	C_{13} H_9 Ag N_2 O S	C_{14} H_{10} Ag N_3 O S_2
Formula weight	349.15 g/mol	408.24 g/mol
Temperature	100(2) K	293(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Orthorhombic	Triclinic
Space group	*P n a* 2_1	*P -1*
Unit cell dimensions	a = 27.2079(9) Å	a = 6.0975(2) Å
	b = 6.0833(2) Å	b = 8.7626(4) Å
	c = 7.5732(2) Å	c = 14.6204(6) Å
	α = 90°	α = 95.010(2)°
	β = 90°	β = 100.1270(10)°
	γ = 90°	γ = 90.578(2)°
Volume	1253.47(7) $Å^3$	765.80(5) $Å^3$
Z	4	2
Density (calculated)	1.850 g/cm^3	1.770 g/cm^3
Absorption coefficient	1.761 mm^{-1}	1.589 mm^{-1}
F(000)	688	404
Crystal size	0.10 x 0.16 x 0.21 mm^3	0.18 x 0.23 x 0.45 mm^3
Theta range for data collection	3.00 to 30.57°	1.42 to 25.00°
Index ranges	-36<=h<=38, -7<=k<=8, -10<=l<=10	-7<=h<=7, -10<=k<=10, -17<=l<=17
Reflections collected	12897	12502
Independent reflections	3773 [R(int) = 0.0273]	1060 [R(int) = 0.0314]
Completeness to theta = 30.57°	99.8%	39.1%
Absorption correction	Multiscan	Multiscan
Max. and min. transmission	0.8410 and 0.7040	0.7630 and 0.5350
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	3773 / 1 / 163	1060 / 0 / 190
Goodness-of-fit on F^2	0.971	1.238
Final R indices [I>2sigma(I)]	R1 = 0.0228, wR2 = 0.0580	R1 = 0.0143, wR2 = 0.0382
R indices (all data)	R1 = 0.0244, wR2 = 0.0589	R1 = 0.0144, wR2 = 0.0382
Largest diff. peak and hole	0.549 and -0.778	0.159 and -0.163